Modeling & Simulation

Data Analysis and Modeling & Simulation for the Chemical Sciences

Project Description

Almos every scientific activity at Los Alamos involves data analysis and modeling. From a chemical sciences point of view, such work transforms “raw” data into a form that provides useful information that is predictive, confirmatory, or exploratory.

The key to understanding the world around us is the ability to put the chemical data we collect into a meaningful context with respect to the problem at hand. Data analysis and modeling and simulations provide powerful tools to help accomplish that task. This capability, when combined with the powerful information science and technology resources of the Laboratory, provides critical contributions to many other research efforts.

Combined with measurement and detection, data analysis and modeling form the core of the chemical-sciences contribution to the Science of Signatures effort at the Laboratory.

Capabilities

Developing remote-sensing devices for nuclear nonproliferation and other needs, such as detecting improvised explosive devices.

Performing process modeling that scales from bench-top chemical kinetic and thermodynamic experiments to pilot- and plant-sized programs.

Simulating new chemicals/materials with tailored properties for diverse applications.

Analyzing chemical rate for complex modeling needs.

Performing chemical-sciences data analysis and modeling for nuclear forensics.

Carrying out high-throughput high-data genome sequencing.

Conducting data analysis and modeling of secured systems.

Analyzing high explosive data and performing thermodynamic and kinetic modeling.

Developing pattern-recognition algorithms to detect trace species in analytical chemistry data.

Research and Technology Development Areas

- Developed KIVA, a code used to analyze chemically reacting flows with sprays. KIVA uses ALE (Arbitrary Langrangian Eulerian) methodology on a staggered grid,

and it discretizes space using a finite-volume technique. The code uses implicit time advancement, except for the advective terms, which are cast in an explicit but second-order monotonicity-preserving manner. Convection calculations can be subcycles in desired regions to avoid restricting the time step caused by Courant conditions. KIVA applications include performing low and combustion modeling in spark-ignition diesel engines and gas turbines, analyzing flows in automotive catalytic converters, designing fire-suppression systems, and designing pulsed detonation propulsion systems.

- Worked with Proctor and Gamble on computer codes used for predictive modeling. Such codes are part of the Los Alamos Computational Fluid Dynamics Library —software packages that include computer-modeling codes developed to solve problems related to the dynamic behavior of materials. These codes can model all types of behaviors, from rain falling through the air to the transport of coal slurry through piping to the initial mixing of coffee and milk.
- Developed CartaBlanca, an advanced object-oriented simulation software package that offers researchers modeling and simulation capabilities in a number of disciplines. Written in the “developer friendly” Java language, it enables computer code developers to simulate complex nonlinear effects such as airflow through a turbo booster, blast effects on buildings, or heat transfer along a semiconductor. Because it is a Java-based software package, the code is much easier to use, manipulate, and modify than codes based on programming languages such as FORTRAN or C++. Applications for chemical sciences include computational fluid dynamics, fluid/solid interactions, and pharmaceutical processing. CartaBlanca received an R&D 100 Award in 2005.
- Developing and fielding new types of remote-sensing instruments designed to detect spectral or optical signatures of importance in proliferation detection and other applications such as battlefield threats and intelligence gathering. We use the latest technology in data acquisition and geographical information systems to execute field campaigns with high efficiency and enable the rapid transformation of sensor data to intelligence assessment, in some cases in near real time. Theoretical research is aimed at developing detection algorithms (for gas chemicals, solid materials, and others) to extract signals from high levels of background clutter, using both conventional techniques based on matched filtering and machine learning methods to improve detection under specialized conditions. We also make optimal use of chemical and physical intuition to identify new signatures for proliferation activity, which feeds back into instrument design.
- Developing new ways to identify and locate clandestine sites dedicated to nuclear processing and purification of plutonium and uranium. Efforts include identifying new chemical signatures and observables, increasing the sensitivity of existing signatures, and expanding the range of temporal resolution of signature detection for nonproliferation efforts.
- Performing chemical-sciences data analysis and modeling for nuclear forensics. Modeling teams use radiochemistry fingerprints and prompt-signal data to reverse engineer exact weapons design while data crunching yields fingerprints of initial fuel and weapon type. Los Alamos originally implemented nuclear forensics in 1945, when Manhattan Project pioneers analyzed debus from the first nuclear explosion. Today nuclear forensics is a mature science, based on the analysis of debris from over a thousand U.S. nuclear tests; extensive research and design in all aspects of nuclear weaponry; modeling of nuclear performance with some of the fastest supercomputers in the world; and use of unique radiological and nuclear

facilities such as Technical Area 48, the Chemistry and Metallurgy Research building, and the Plutonium Facility.

LANL Facilities and Resources

- Center for Integrated Nanotechnologies: Scientists at this center develop the scientific principles that govern the design, performance, and integration of nanoscale materials.
- Strategic Computing Complex: Also known as the Nicholas C. Metropolis Center for Modeling and Simulation, this complex houses supercomputers that support the calculation, modeling, simulation, and visualization of complex nuclear weapons data in support of the Stockpile Stewardship Program. The complex includes a Data Visualization Corridor, which enables scientists to view the models and simulations created by the supercomputers. The Data Visualization Corridor includes a Powerwall Theater and a five-sided CAVE Immersive Laboratory, as well as desktop visualization and collaborator capabilities.
- Exascale Co-design Center for Materials in Extreme Environments: Exascale computing presents an enormous opportunity for solving some of today's most pressing problems, including clean energy production, nuclear reactor lifetime extension, and nuclear stockpile aging. At their core, each of these problems requires the prediction of material response to extreme environments. This center's objective is to establish the interrelationship between software and hardware required for materials simulation at the exascale while developing a multiphysics simulation framework for modeling materials subjected to extreme mechanical and radiation environments.
- Information Science & Technology Institute: This institute covers a range of fields, including information science and technology, computer science, computational science, and applied mathematics. Topic areas include extreme-scale data management, high-performance computing, data-intensive computing, computational co-design, reliability and resilience at scale, algorithms and methods (including informatics), and multicore and hybrid computing.

Key Personnel at LANL

- Joel Kress: Physics and chemistry of materials
- Mark Schraad: Computational fluid dynamics
- Hugh Selby: Nuclear forensics

Sponsors, Funding Sources, or Agencies

- Department of Homeland Security
- Department of Energy
- Department of Defense

Awards

- 2005 R&D 100 Award for CartaBlanca

Publications

C.E. Starrett, J. Clérouin, V. Recoules, J.D. Kress, L.A. Collins, and D.E. Hanson, “Average atom transport properties for pure and mixed species in the hot and warm dense matter regimes,” Physics of Plasmas 19(10) (2012).

L.A. Collins, J.D. Kress, and D.E. Hanson, “Reflectivity of warm dense deuterium along the principal Hugoniot,” Physical Review B - Condensed Matter and Materials Physics 85(23) (2012).

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David E. Hanson, Lee A. Collins, Joel D. Kress, and Michael P. Desjarlais, “Calculations of the thermal conductivity of national ignition facility target materials at temperatures near 10 eV and densities near 10 g/cc using finite-temperature quantum molecular dynamics,” Physics of Plasmas 18(8) (2011).

J.D. Kress, James S. Cohen, D.P. Kilcrease, D.A. Horner, and L.A. Collins, “Quantum molecular dynamics simulations of transport properties in liquid and dense-plasma plutonium,” Physical Review E - Statistical, Nonlinear, and Soft Matter Physics 83(2) (2011).

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D.A. Horner, J.D. Kress, and L.A. Collins, “Effects of metal impurities on the optical properties of polyethylene in the warm dense-matter regime,” Physical Review B - Condensed Matter and Materials Physics 81(21) (2010).

Michael R. Salazar, Joel D. Kress, J. Michael Lightfoot, Bobby G. Russell, Wayne A. Rodin, and Lorelei Woods, “Low-temperature oxidative degradation of PBX 9501 and its components determined via molecular weight analysis of the Poly[ester urethane] binder,” Polymer Degradation and Stability 94(12), 2231–2240 (2009).

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